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The Energy Dispersion of the Chain Band in YBa2Cu3O6+y, and Its Effect on the Cu(2) NQR Frequency

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Abstract

The energy dispersion of the chain band has been determined in the framework of the Hubbard model. The results are in agreement along the T-S and T-Y lines of the Brillouin zone with photoemission data. The amount of d3z2-r2 states is zero at y = 0 and increases to 10% at y = 1. The admixture is due to the hybridization of Cu(1) dy2−z2 states with Cu(2) d3z2-r2 states via apical oxygen. The effect of this admixture on the NQR Frequency of Cu(2) is discussed.

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Keywords

Band dispersion, Chain band, d3z2-r2 states, Electron correlation, NQR